A New Acylated Flavonoid from Anaphalis aureo-punctata

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Abstract: A new acylated flavonoid glycoside, 3-O-kaempferol-3-O-acetyl-6-O-(p-coumaroyl)- β -D-glucopyranoside **1** was isolated from the whole plant of *Anaphalis aureo-punctata*. The structure was established by spectral methods.

Keywords: *Anaphalis aureo-punctata*, flavonoid, 3-O-kaempferol-3-O-acetyl-6-O-(*p*-coumaroyl)β-D-glucopyranoside.

The genus *Anaphalis* (Compositae) consists of about 80 species distributed throughout the world. Among them, *Anaphalis morrisonicola* showed significant antitumor activity¹. In order to find active constituents, phytochemical studies on *Anaphalis aureo-punctata* were carried out and a new acylated flavonoid **1** was isolated from the alcoholic extract of the whole plant. In this paper, we report the structural elucidation of the compound **1**.

Figure 1 The key correlation of **1** in HMBC ($H \rightarrow C$)



Compound 1 was obtained as a yellow crystalline powder, $[\alpha]_{D}^{21}$ -53.0 (c, 2.3, CH₃OH). It was established to have a molecular formula C₃₂H₂₈O₁₄, which was deduced by FAB-MS (*m*/*z* 659 [M+Na]⁺, 643 [M+Li]⁺) and ¹³C NMR data including DEPT technique. The analysis of ¹H and ¹³C NMR spectra (**Table 1**) suggested that 1 was a kaempferol (*p*-coumaroyl)glycoside². The singlet at δ 2.03 (3H) indicated the presence of an acetyl group in this compound. The large coupling constant between the H- α and H- β (J=16.0 Hz) showed the E-configuration for the double

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bond.

The HMBC cross peak at δ 5.53/133.0 (H-1" /C-3) revealed the connection point between the sugar moiety and aglycone to be at C-3. The correlations from the acetyl protons (δ 2.03) and H-3" (δ 4.71) to the acetyl carbonyl (δ 169.8), from H- β (δ 7.37) and H-6" (δ 4.00) to the coumaroyl carbonyl (δ 166.0) suggested the acetoxy group at C-3" and the *p*-coumaroyloxy group at C-6"³. The key correlations of HMBC were showed in **Figure 1**. Consequently, the structure of **1** was established.

Table 1 $~^{1}{\rm H}$ (400 MHz) and ^{13}C (100.6 MHz)NMR data of compound 1 (DMSO-d_6 , TMS, δ ppm)

No.	$\delta_{\rm H}({\rm J~Hz})$	δ_{C}	DEPT	No.	$\delta_{\rm H}({\rm J~Hz})$	$\delta_{\rm C}$	DEPT
2		156.8	С	3"	4.71 d (9.2, 9.0)	70.9	СН
3		133.0	С	4"	3.55 d (9.0, 9.0)	71.5	CH
4		177.4	С	5"	3.70 m	74.2	CH
5		161.3	С	6"	4.00 d (5.0)	62.0	CH_2
6	6.17 d (1.8)	98.9	CH	coumaroyl			
7		164.3	С	COO		166.0	С
8	6.39 d (1.8)	93.8	CH	α	6.10 d (16.0)	113.5	CH
9		156.5	С	β	7.37 d (16.0)	144.9	СН
10		104.0	С	1""		125.0	С
1'		120.8	С	2''', 6'''	7.38 d (8.4)	130.2	CH
2' 6'	8.00 d (8.8)	130.9	CH	3"', 5"'	6.80 d (8.4)	115.9	СН
3' 5'	6.89 d (8.8)	115.2	CH	4"'		159.9	С
4'		160.1	С	3"-Acetyl			
glu				COO		169.8	С
1"	5.53 d (7.8)	101.0	CH	CH ₃	2.03 s	20.9	CH_3
2"	3.37 d (7.8, 9.2)	73.5	СН				

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